Potential energy surfaces and dynamics of chemical reactions

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The recent theoretical work directed toward the understanding of elementary chemical reactions is discussed. First, we concentrate on the modelling of the relevant potential energy surfaces with emphasis on processes which involve more than one electronic state. Then, we overview the results of some specific dynamic studies. These include three-dimensional wavepacket calculations of transition state resonances for triatomic systems with and without consideration of nondiabatic effects, in addition to classical and quantum rate constant calculations of four-atom atmospheric reactions with relevance in the ozone chemistry. We conclude with some studies that could be undertaken in the future.

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Chemical reaction information retrieval – sources and problems from a user's perspective

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Searching for reactions of organic compounds is one of the most intricate tasks in chemical information retrieval, because it usually incorporates (sub)structures, keywords, and numeric data, individually or in any conceivable combination. This is therefore demanding not only on the user with regards to query formulation and evaluation of results, but even more so on retrieval systems and databases. By contrast to compound or literature database, reaction databases can be grouped into two categories: intellectually or algorithmically selected sources (''reaction type'' databases), and ''comprehensive'' sources (''individual reaction'' databases). Even the databases in the latter category, however, are not nearly as large (by number of records) or comprehensive as compound or literature databases; therefore, deductions and conclusions based on analogy are significantly more important in reaction retrieval than elsewhere. Interfaces between programs for synthesis planning or reactivity prediction and the large reaction ''data pools'' are not as well established as necessary to provide improved tools for organic chemists. As illustrated by an attempted very simple type classification of reaction queries, both categories of databases mentioned before play different, but similarly important roles in supporting execution of chemical preparations, synthesis planning, and chemical reactivity prediction.

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